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HYDROGEN GENERATION FOR SELECT FTS SCENARIOS

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K Basins Closure Project
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APPENDIX A
FATE Computer Code

A.1 General

The FATE™ 2.0 Computer Code is used for this analysis. FATE is the successor code to the HANSF computer program used for previous sludge analyses in HNF-22075, Rev. 0.

FATE stands for Facility Flow, Aerosol, Thermal, and Explosion Model, for PCs and workstations [Plys and Lee, 2004]. FATE 2.0 is used for design, off-normal, and accident analyses of nuclear and chemical facilities. FATE 2.0 is the successor to computer codes used extensively for design and safety analyses for U. S. Department of Energy projects at the Hanford site and elsewhere (HADCRT for Tank Farms, Waste Treatment Plant, WESF, PFP; HANSF MCO and HANSF Sludge for Spent Nuclear Fuel and sludge, T Plant).

General capabilities of FATE 2.0 include:

- Fire model: Define burn rate and yields; Smoky layer model; Propagation of smoke in stratified layers throughout facility; Aerosol transport with smoky layers; Aerosol settling from smoky layer to lower layer and embedded surfaces.
- Multiple-compartment thermodynamics and general species: Facility rooms have separate pressure, temperature, and composition; Compound property libraries are input; Tracking of condensed, gaseous, and aerosol species.
- Facility nodalization and flow: Compartments are connected in arbitrary topology by flow paths; Flows are pressure-driven, density-driven counter-current, and diffusional.
- Aerosol behavior: Aerosol coagulation, sedimentation, transport with flow; Deposition on bends and filters; Deposition by condensation; Aerosol formation by boiling and fog.
- Heat transfer: Convection of liquids and gases to structures with internal temperature distributions; Linking for 2D and 3D heat transfer; Condensation.

- Flammability and combustion of gases, vapors, and aerosols: Any input compound may participate; examples include solvent vapors, hydrogen, and U metal or hydride aerosols.
- Entrainment of deposits to form aerosols: Powder, liquid, and sludge waste may be entrained by combustion or flow.
- Thermal radiation networks: View factor models and automatic network balancing.
- Event-oriented simulation: Intervention criteria and actions for scenario evolution.
- Sources and time-dependent conditions. Prescribe liquid, gas, and aerosol source histories and environmental conditions with time.
- Nuclear fuel and sludge models including chemical reactions.

FATE is owned and licensed by FAI. FATE is created and maintained under the FAI Quality Assurance Program (10CFR50 App. B & ISO 9001 compliant).

A.2 FATE and HANSF Utilization at Hanford

Before the current computer code revision to FATE 2.0, HANSF was the name given to the models specifically written for the Hanford Spent Nuclear Fuel Project (SNFP) that resided within a generic facility model, HADCRT. HADCRT was the name of the computer code containing all generic models and capable of invoking SNFP multi-canister overpack (MCO) and sludge specific models. Baseline quality assurance (QA) versions with the common platform were created in this order:

1) HADCRT 1.4 for generic models (*Fuel Cycle Facility Source Term Model HADCRT 1.4: User's Manual (FAI/02-50))*, [Plys, et al., 2002a];
2) HADCRT 1.4A for sludge models (*HANSF/SLUDGE Computer Program User's Manual, FAI/02-13),* [Plys, et al., 2002b];
3) HADCRT 1.4B for MCO models (*Hanford Spent Nuclear Fuel Process and Safety Analysis Model HANSF/MCO 1.4: User's Manual (HADCRT 1.4B)),* [Plys, et al., 2002c]; and

4) FATE 2.0, current computer code version (*FATE 2.0: Facility Flow, Aerosol, Thermal, and Explosion Model, Improved and Combined HANSF and HADCRT Models),* [Plys, et al., 2004].

Depending on whether MCO-specific models or sludge-specific models are activated, the computer program was also called HANSF, HANSF/MCO, or HANSF/SLUDGE. If neither model is invoked (i.e., only generic models are used), the computer program was called HADCRT; this name will be used here to describe previous usage.

FATE Generic models may be used to model normal processes, operational transients, and accidents at fuel cycle facilities, such as Hanford K basins, the Canister Storage Building (CSB), tank farm facilities including underground waste tanks, pits, and multi-room vaults, the future Waste Treatment Plant (WTP), and other facilities such as T-Plant, Waste Encapsulation and Storage Facility (WESF), Waste Receiving and Processing (WRAP) plant, and Plutonium Finishing Plant (PFP). A typical use is to predict radiological consequences of an accident involving combustion, including attenuation of radionuclides within the facility (the so-called leak path factor).

Example analyses include double-shell tank gas release (tank bump) analysis (*Hanford Waste Tank Bump Accident and Consequence Analysis* [Epstein, et al., 2000]); combustion in double-contained receiver tanks (*Combustion Accident Analysis for Double-Contained Receiver Tanks (DCRT) 244-S and 244-TX* [Siciliano and Puigh, 1999]); and combustion in the WTP (*Topical Report on the Management of Risks Posed by Explosive Hazards Present at the RPP-WTP* [BNFL and FAI, 1999]).

Recent large-scale analyses have been conducted with HADCRT for the Hanford WTP (*Analysis of a HLW Process Vessel Hydrogen Deflagration Using HADCRT Computer Code*; *Analysis of HLW Melter Unplanned Pour Using HADCRT Computer Code*; *Beyond Design Basis Event - LAW Melter Offgas Release Event Using HADCRT Computer Code* [Crowe and Lanning, 2002a; 2002b; and 2003]). The first analysis considered a sudden leak of low-activity waste (LAW) melter offgas into the melter facility, tracked hazardous gases and radioactive aerosols throughout the facility including the heating, ventilation, and air conditioning (HVAC) system, and was used to predict leakage into occupied areas and the environment. The second predicted temperatures, pressures, and flows resulting from hydrogen combustion in process vessels, including the vessel vent system and HVAC systems for the high-level waste (HLW) facility. The third analyzed the impacts of an unplanned pour from the HLW melter, which include local heating of concrete walls and floor by radiation and convection, local gas temperatures and pressurization, and maximum temperatures seen by downstream high-efficiency particulate air (HEPA) filters.

MCO models were developed to include specific models for fuel behavior inside an MCO container for shipping, processing, and storage of Hanford Site spent nuclear fuel. These include models for fuel oxidation, hydrogen production, hydrate decomposition, ice formation, and numerous other phenomena pertinent to MCO process analyses. Together with the generic capability, the code is also capable of estimating the aerosol source term from accidents, such as depressurization of an MCO or from hydrogen combustion. Example analyses conducted with the MCO models are *Simulation of Normal and Off-Normal Multi-Canister Overpack Behavior* [Plys, et al., 1998] and *Thermal Analysis of Cold Vacuum Drying of Spent Nuclear Fuel* [Piepho, 2000]. In Plys, et al. [1998], a "cradle to grave" analysis of MCO behavior from vacuum drying through dry storage was conducted. Analyses from Piepho [2000] form the basis for the SNFP safety analysis report.

Sludge models were created to model thermal and chemical properties of Hanford Site spent nuclear fuel sludge within the integral model framework. This allows a complete analysis of behavior internal to sludge, such as oxidation, heat generation, hydrogen generation, and prediction of the sludge temperature profile, coupled with behavior external to sludge, such as calculation of pressures and gas concentrations in a sludge container, exchange flows between a sludge container and a facility, and gas concentrations throughout a facility. Using the same nodalization, the calculations can include accident analysis such as combustion and depressurization, with creation, transport, and deposition of aerosols, providing estimates of the aerosol source term, facility leak path factor, and source to the environment. Analyses of sludge container behavior in transport and at T Plant are described in *Independent Calculation for Hanford Sludge Transportation and Storage (FAI/02-11)* [Plys, 2002].

FATE can be used for design and scoping evaluations as well as accident analyses, and indeed, it is common to first create a design via scoping and then, via straightforward new inputs, specify an accident scenario. An example of this range of capability is found in *Accident and Thermal Analysis for Storing K East Basin Sludge at T Plant* [Fuller, 2003], where the sludge model was used to simulate various open port arrangements for a sludge container placed in a cell at T Plant. A design was found which would prevent the accumulation of a flammable composition in the container, considering simultaneously the buildup of flammable gases in the cell; it was also able to predict the annual water loss rate. This input file was then extended to consider consequences of hydrogen combustion and entrainment from the container, and exposure of the container in a transfer cask to an external fire.

A.3 References

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